# Fourier Neural Operator: Learning Solution Operators in Spectral Space

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# Overview

# Outline

# Learning Objectives

- Understand the connection between CNNs and kernel operators
- Master Fourier Transform fundamentals for neural operators
- Learn the FNO architecture: spectral convolution layers
- Implement FNO for 1D Burgers equation
- Apply FNO to 2D Darcy Flow problem
- Explore mesh independence and super-resolution capabilities

Open Notebook: FNO

# The Central Challenge

We've seen how DeepONet learns operators by decomposing them into branch-trunk architectures.

**But there's a deeper question**

What if **physics itself suggests the right representation**?

For 50+ years, **spectral methods** based on Fourier transforms have dominated computational physics because:

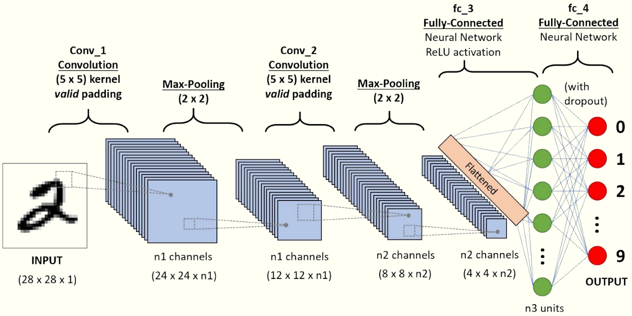
- Many PDEs simplify in Fourier space (convolution $\rightarrow$ multiplication)
- Derivatives become algebraic: $\mathcal{F}\left(\frac{\partial u}{\partial x}\right) = ik\hat{u}(k)$
- Global information propagates naturally

**The FNO insight:** Learn operators *in Fourier space* rather than physical space.

# Convolutional Neural Networks: The Foundation

CNNs apply **local** kernels to extract features:

$$(f * g)(x) = \int_{\text{local}} f(x')g(x - x')dx'$$




CNN architecture with convolutional and pooling layers.

## Key properties:

# Kernel Operators: The General Form

A **kernel operator** maps functions to functions:

$$\mathcal{K}(v)(x) = \int_{\Omega} \kappa(x, x')v(x')dx'$$

where $\kappa(x, x')$ is a **learned kernel**.

**Types of kernels:**

1. **Standard convolution:** $\kappa(x, x') = k(x - x')$ (local, translation-invariant)
2. **Graph operators:** $\kappa$ defined on graph edges
3. **Fourier operators:** $\kappa$ learned in spectral space (global, efficient)

**Why Fourier?**

Convolution in physical space = multiplication in Fourier space!

# Outline

# The Fourier Transform

**Mathematical Definition:**

The Fourier Transform decomposes a function into sinusoidal components:

$$\hat{u}(k) = \mathcal{F}(u)(k) = \int_{-\infty}^{\infty} u(x)e^{-ikx}dx$$

**Inverse Fourier Transform:**

$$u(x) = \mathcal{F}^{-1}(\hat{u})(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{u}(k)e^{ikx}dk$$

**Key insight:** Any function can be written as:

$$u(x) = \sum_{k} \hat{u}_k e^{ikx}$$

where $\hat{u}_k$ are **Fourier coefficients** (complex weights) and $e^{ikx}$ are basis functions.

# Essential Properties of Fourier Transform

## 1. Derivatives become multiplication

$$\mathcal{F}\left(\frac{\partial u}{\partial x}\right) = ik\hat{u}(k)$$

## 2. Convolution becomes multiplication (Convolution Theorem)

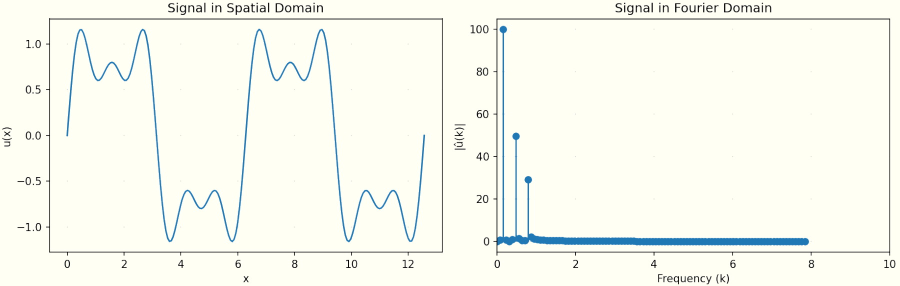
$$\mathcal{F}(u * v) = \mathcal{F}(u) \cdot \mathcal{F}(v)$$

## 3. Parseval's theorem (Energy conservation)

$$\int |u(x)|^2 dx = \int |\hat{u}(k)|^2 dk$$

**Computational advantage:** FFT is $O(N \log N)$, far cheaper than dense convolution $O(N^2)$.

# Fourier Decomposition: Visualization




Fourier decomposition: A function (left) is represented as a sum of weighted sinusoids (middle), with most energy concentrated in low frequencies (right).

**Key observation:** Most energy concentrated in low frequencies.
**FNO exploits this:** Learn weights only for low-frequency modes ($k_{\max} \approx 12 - 16$), discard high frequencies.

# Outline

# The Core Idea

Instead of learning in physical space, **learn in Fourier space**:

$$v_{t+1}(x) = \sigma\left(W v_t(x) + \mathcal{K}(v_t)(x)\right)$$

where the kernel operator $\mathcal{K}$ is parameterized in Fourier space:

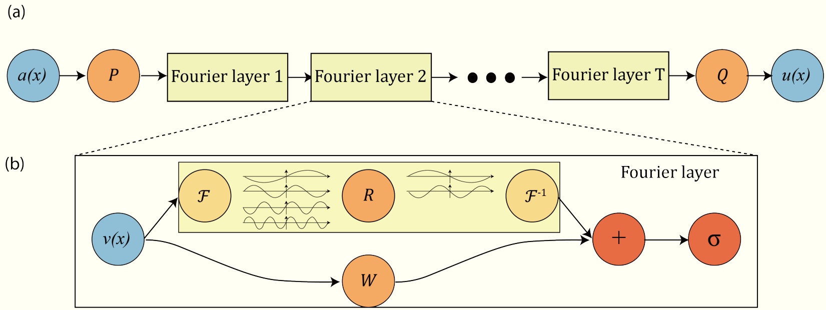
$$\mathcal{K}(v)(x) = \mathcal{F}^{-1}\left(R_\phi \cdot \mathcal{F}(v)\right)(x)$$

Here, $R_\phi$ are **learnable weights** in Fourier space.

## The FNO workflow

$$\text{Input } u(x) \xrightarrow{\text{FFT}} \text{Fourier Space} \xrightarrow{\text{Learn } R_\phi} \text{Fourier Space} \xrightarrow{\text{IFFT}} \text{Output}$$

# Complete FNO Architecture




Fourier Neural Operator architecture.

**Architecture consists of:**

- **Lifting:** $P(u) \to v_0$ (embed input to high-dimensional space)
- **Fourier Layers:** $v_{t+1} = \sigma(Wv_t + \mathcal{K}(v_t))$ (4 layers)
- **Projection:** $Q(v_4) \to$ output (map back to output space)

# Spectral Convolution Layer

Each Fourier layer performs three operations:

1. **FFT:** $\hat{v} = \mathcal{F}(v)$
2. **Linear transform (truncated):**

$$\hat{v}_{\text{out}}[k] = R_\phi[k] \cdot \hat{v}[k] \quad \text{for } k \leq k_{\max}$$

3. **IFFT:** $v_{\text{out}} = \mathcal{F}^{-1}(\hat{v}_{\text{out}})$

**Key design choice**

Only keep low-frequency modes ($k_{\max} \approx 12 - 16$), discard high frequencies. **Why?** Most signal energy in low frequencies + acts as implicit regularization.

# Spectral Convolution: Mathematical Details

For 1D problems:

$$\text{SpectralConv1d}(v) = \mathcal{F}^{-1}\left(R \cdot \mathcal{F}(v)[:k_{\max}]\right)$$

For 2D problems:

$$\text{SpectralConv2d}(v) = \mathcal{F}^{-1}\left(R_1 \cdot \mathcal{F}(v)[:k_1, :k_2] + R_2 \cdot \mathcal{F}(v)[-k_1 :, :k_2]\right)$$

**Learnable parameters:** $R \in \mathbb{C}^{c_{in} \times c_{out} \times k_{\max}}$

**Skip connections:** Standard 1x1 convolution in parallel

$$v_{\text{out}} = \sigma(\text{SpectralConv}(v) + Wv)$$

# Outline

# The 1D Viscous Burgers Equation

**Problem Formulation:**
The 1D viscous Burgers equation models shock wave propagation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}, \quad x \in [0, 2\pi], t \in [0, T]$$

with periodic boundary conditions and initial condition $u(x, 0) = u_0(x)$.

**Operator learning task:** Learn the mapping

$$\mathcal{G} : u_0(x) \mapsto u(x, T)$$

from initial condition to solution at time $T = 1$.

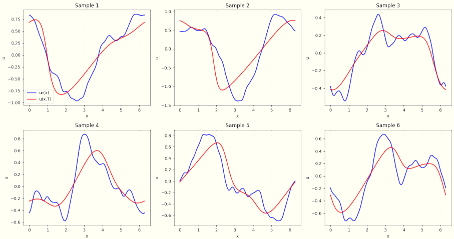
**Dataset:** 1024 training samples from varied initial conditions, solved using spectral methods.

**The physics:**

- **Nonlinear advection:** $u\frac{\partial u}{\partial x}$
- **Viscous diffusion:** $\nu\frac{\partial^2 u}{\partial x^2}$
- Competition creates shock waves
- Periodic boundary conditions

**Why this problem:**

- Prototype for nonlinear PDEs
- Captures shock formation
- Tests operator learning on complex dynamics




Sample initial conditions (blue) and evolved solutions (red) showing shock formation.

# 1D FNO Architecture and Training

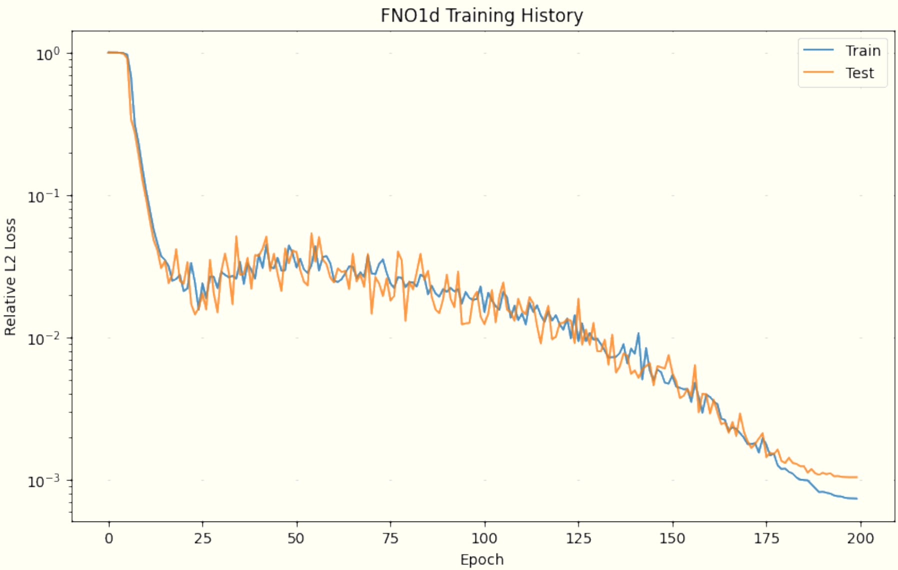
**Model Configuration:**

- **Input:** $(u_0(x), x)$ at $m = 2048$ points (subsampled to 512)
- **Fourier modes:** $k_{\max} = 16$
- **Hidden width:** $w = 64$
- **Layers:** 4 Fourier layers with skip connections
- **Activation:** GELU
- **Parameters:** $\sim$287K

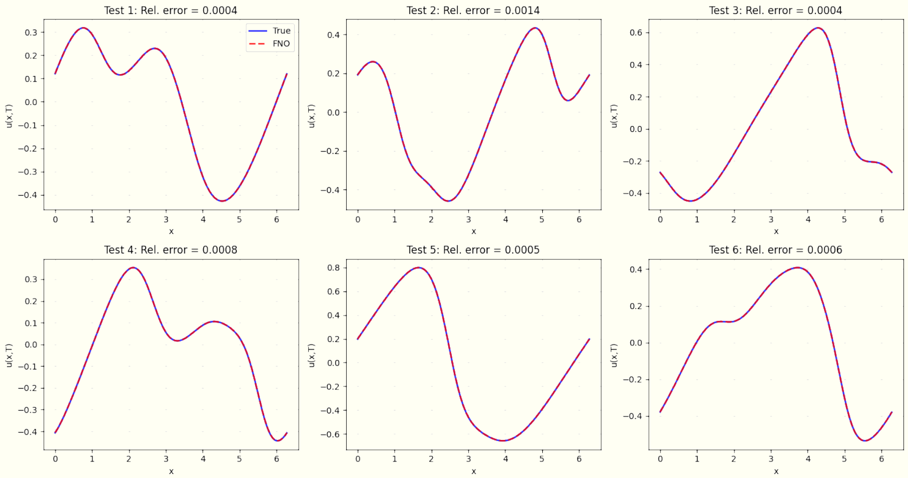
**Training Configuration:**

- **Loss:** Relative $L^2$ loss: $\frac{\|u_{pred} - u_{true}\|_2}{\|u_{true}\|_2}$
- **Optimizer:** Adam with OneCycleLR scheduler
- **Training samples:** 1000
- **Test samples:** 100
- **Epochs:** 200

# Burgers Equation: Training Results



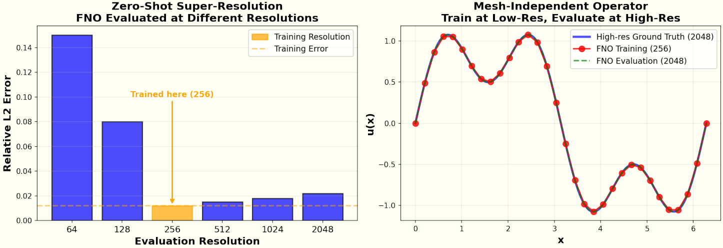
# Burgers Equation: Prediction Quality




FNO predictions (red dashed) vs. true solutions (blue) for test cases.

**Key results:**

# Zero-Shot Super-Resolution




Training at 512 resolution, evaluating at 2048 resolution (4x upsampling).

## Mesh Independence

- **Train:** 512 grid points
- **Test:** 2048 grid points (4x refinement)
- **Result:** Maintains accuracy at higher resolution!

**Why this works:** FNO learns in Fourier space (continuous representation), not tied to specific discretization.

# Outline

# The 2D Darcy Flow Equation

**Problem Formulation:**

The 2D Darcy flow equation models steady-state flow in porous media:

$$-\nabla \cdot (a(x,y)\nabla u(x,y)) = f(x,y), \quad (x,y) \in [0,1]^2$$

with zero boundary conditions: $u|_{\partial\Omega} = 0$.

**Operator learning task:** Learn the mapping

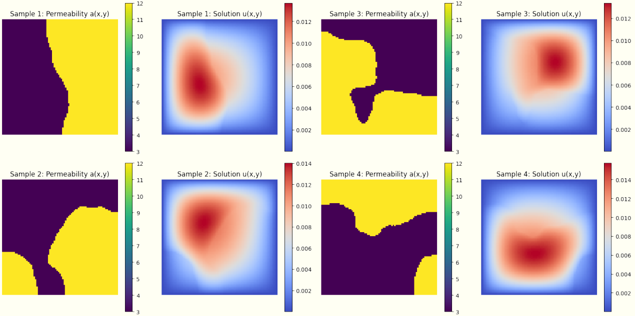
$$\mathcal{G} : a(x,y) \mapsto u(x,y)$$

from permeability coefficient $a$ to pressure/hydraulic head $u$.

**Physical interpretation:**

- $a(x,y)$: permeability field (how easily fluid flows)
- $u(x,y)$: pressure field
- $f(x,y)$: source term (set to 1)

# Darcy Flow: Dataset and Physics




Left: Permeability fields $a(x, y)$ (input). Right: Pressure fields $u(x, y)$ (output).

**Dataset characteristics:**

# 2D FNO Architecture

**Model Configuration:**

- **Input:** $(a(x,y), x, y)$ at $81 \times 81$ grid
- **Fourier modes:** $k_{\text{max}} = 12$ (both x and y directions)
- **Hidden width:** $w = 32$
- **Layers:** 4 Fourier layers
- **Parameters:** $\sim$130K

**Spectral Convolution 2D:**

$$\text{FFT2} \rightarrow \text{Multiply modes } [:12, :12] \text{ and } [-12:, :12] \rightarrow \text{IFFT2}$$

**Why two weight matrices?** Due to symmetry of real FFT (rfft2), we need weights for both lower and upper frequencies.

# Darcy Flow: Training Configuration

**Training Setup:**

- **Loss:** Relative $L^2$ loss in 2D
- **Optimizer:** Adam with step decay (StepLR)
- **Learning rate:** 0.001 with decay every 50 epochs
- **Batch size:** 20
- **Epochs:** 200 (500 in original paper)

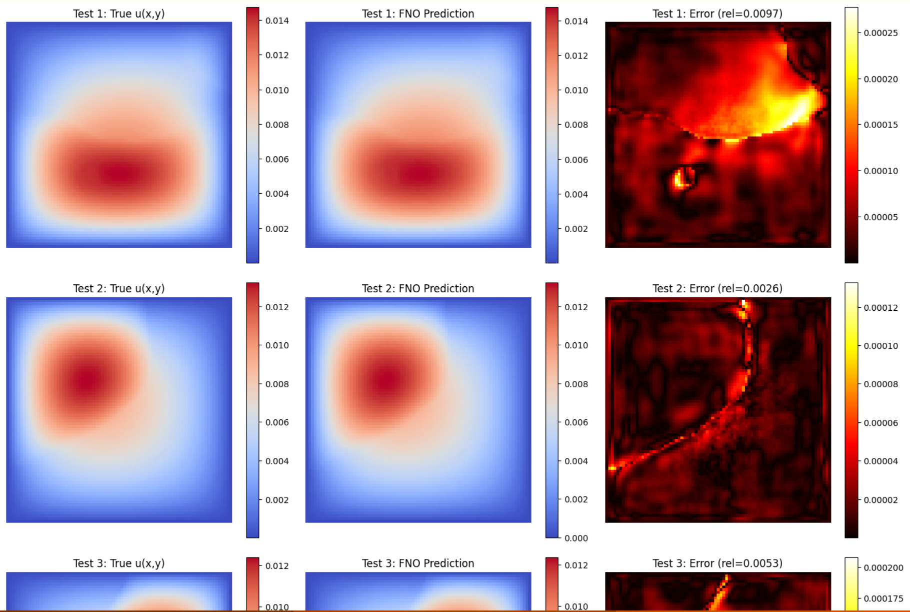
**Data Normalization:**

- Input permeability: Unit Gaussian normalization
- Output pressure: Unit Gaussian normalization
- Decode predictions before computing loss

**Important**

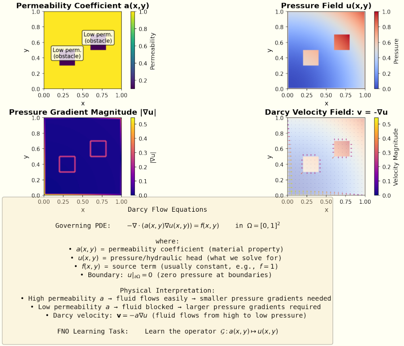
Normalize data for stable training, but always compute loss on physical quantities!

# Darcy Flow: Results and Analysis



## Why circular patterns?

- Elliptic PDE creates smooth distributions
- Source term $f = 1$ uniformly
- Zero boundary conditions
- Low permeability $\rightarrow$ high pressure




Physical interpretation: Permeability variations create pressure "bubbles".

## Error patterns show:

- Higher errors near boundaries
- Errors in steep gradient regions
- Suggests need for more training

**Key takeaway:** The patterns are physically correct - FNO learned the right physics!

# Outline

# What Makes FNO Special?

## 1. Mesh Independence

- Train on one resolution, evaluate on any resolution
- Works because we learn in Fourier space (continuous representation)
- Discretization is only for FFT computation

## 2. Computational Efficiency

- FFT: $O(N \log N)$ vs dense convolution $O(N^2)$
- Once trained: milliseconds per evaluation
- Traditional solver: seconds to minutes

## 3. Global Receptive Field

- Fourier modes capture global information
- No need to stack many layers for long-range dependencies
- Contrast with CNNs: local receptive fields

# Physics-Informed Design

**Why Fourier space is natural for physics:**

- **50+ years of spectral methods:** Physicists have used Fourier for PDEs since the 1960s
- **Derivatives are algebraic:** $\partial_x \to ik$
- **Convolution theorem:** Simplifies nonlinear terms
- **Natural for periodic BCs:** Exact representation

**Key insight**

FNO doesn't invent a new representation - it uses the one physicists have known works well!

**Low-frequency truncation benefits:**

- **Efficiency:** Most energy in low frequencies
- **Regularization:** Implicit smoothing
- **Generalization:** Avoids overfitting to high-frequency noise

# Limitations and Considerations

## 1. Periodic Boundary Conditions

- Standard FFT assumes periodicity
- Extensions needed for general geometries (Geo-FNO)
- Works perfectly for: Navier-Stokes on periodic domains
- Challenges for: Complex geometries, irregular domains

## 2. Data Requirements

- Need many solved PDE instances for training
- Expensive data generation phase
- Can be mitigated with physics-informed training

## 3. Black Box Nature

- No explicit PDE enforcement during training (standard FNO)
- May violate physical constraints
- Solution: Physics-Informed FNO

# FNO vs DeepONet: Comparison

| Aspect | DeepONet | FNO |
|---|---|---|
| **Architecture** | Branch-Trunk | Spectral Convolution |
| **Space** | Physical | Fourier |
| **Queries** | Arbitrary points | Grid points (FFT) |
| **Best for** | Irregular domains | Periodic domains |
| **Parameters** | More | Fewer |
| **Speed** | Fast | Faster (FFT) |
| **Global info** | Via trunk network | Natural in Fourier |
| **Mesh free?** | Yes | No (needs FFT grid) |

**Key difference:**

- **DeepONet:** Learns basis decomposition in physical space
- **FNO:** Learns multiplication in Fourier space

Both are powerful! Choice depends on:

- Boundary conditions (periodic $\rightarrow$ FNO, irregular $\rightarrow$ DeepONet)
- Query pattern (grid $\rightarrow$ FNO, arbitrary points $\rightarrow$ DeepONet)

# Outline

# Extensions to FNO

## Geo-FNO: Arbitrary Geometries

- Use coordinate transforms to handle non-periodic domains
- Applies Fourier layers in transformed space
- Enables FNO for complex geometries

## Physics-Informed FNO

- Add PDE residual to loss function
- Ensures physical consistency
- Reduces data requirements

## Factorized FNO

- Low-rank approximations for 3D problems
- Reduces memory and computation
- Enables high-resolution 3D operator learning

# U-FNO: Multi-Scale Architecture

**U-Net structure with Fourier layers:**

- **Encoder:** Progressively downsample and increase channels
- **Fourier layers:** At each resolution level
- **Decoder:** Progressively upsample with skip connections

**Advantages:**

- Captures multi-scale physics
- Better for problems with localized features
- Skip connections preserve fine details

**Applications:**

- Turbulence (multi-scale eddies)
- Weather prediction (global + local patterns)
- Material design (micro + macro structures)

# Practical Applications

**Where FNO excels:**

**Fluid Dynamics:**

- Navier-Stokes on periodic domains
- Turbulence modeling
- Weather/climate prediction
- Aerodynamics optimization

**Scientific Computing:**

- Quantum mechanics (Schrödinger)
- Wave propagation
- Heat diffusion
- Reaction-diffusion systems

**Engineering Design:**

- Structural optimization
- Material design
- Electromagnetics
- Acoustic modeling

**Inverse Problems:**

- Parameter identification
- Subsurface imaging
- Medical imaging
- Data assimilation

# Outline

# What We've Learned

## 1. Conceptual Foundation

- CNNs are local kernel operators
- FNO extends to global kernel operators in Fourier space
- Physics naturally lives in spectral domain

## 2. Mathematical Framework

- Fourier Transform decomposes functions into frequency components
- Convolution theorem: multiplication in Fourier space
- Operator parametrization: $\mathcal{K}(v) = \mathcal{F}^{-1}(R_\phi \cdot \mathcal{F}(v))$

## 3. Architecture

- Spectral convolution layers: FFT $\rightarrow$ Learn $\rightarrow$ IFFT
- Skip connections for expressivity
- Mode truncation for efficiency and regularization

# Key Advantages of FNO

1. **Resolution independence:** Train on one grid, evaluate on any grid
2. **Computational efficiency:** $O(N \log N)$ via FFT
3. **Global receptive field:** Captures long-range dependencies naturally
4. **Physics-informed:** Leverages 50+ years of spectral methods
5. **Fast inference:** Once trained, millisecond evaluation
6. **Super-resolution:** Zero-shot upsampling capability

**The paradigm shift**

**Traditional:** Solve each PDE instance numerically
**FNO:** Learn the solution operator once, instant evaluation for any input

# When to Use FNO

## Ideal scenarios:

- **Periodic or translation-invariant problems**
- **Need for resolution independence**
- **Real-time PDE solving**
- **Large-scale parameter sweeps**
- **Multi-query problems:** Same operator, many evaluations

## Consider alternatives when:

- **Complex, non-periodic geometries** (use Geo-FNO or DeepONet)
- **Sparse, irregular data** (DeepONet better)
- **Point-wise queries at arbitrary locations** (DeepONet)
- **Very limited training data** (consider PI-FNO)

# Implementation Tips

## 1. Architecture Choices

- **Fourier modes:** Start with 12-16, adjust based on problem
- **Width:** 32-64 for most problems
- **Layers:** 4 is standard, more for complex operators
- **Activation:** GELU works well (smoother than ReLU)

## 2. Training Strategy

- **Loss:** Relative $L^2$ for scale-invariance
- **Optimizer:** Adam with learning rate scheduling
- **Normalization:** Unit Gaussian for inputs and outputs
- **Epochs:** 200-500 depending on problem complexity

## 3. Validation

- Test on different resolutions (super-resolution check)
- Verify physics consistency (if applicable)

# Resources and Further Reading

**Original Paper:**

- Li et al., "Fourier Neural Operator for Parametric PDEs" (ICLR 2021)
- https://arxiv.org/abs/2010.08895

**Extensions:**

- Geo-FNO: https://arxiv.org/abs/2207.05209
- Physics-Informed Neural Operators: https://arxiv.org/abs/2111.03794
- Neural Operator Review: https://arxiv.org/abs/2108.08481

**Code and Data:**

- Official implementation: https://github.com/neuraloperator/neuraloperator
- Course notebooks: https://github.com/kks32-courses/sciml
- Dataset: https://huggingface.co/datasets/kks32/sciml-dataset

# The Bigger Picture

**From Functions to Operators:**

- Neural Networks $\rightarrow$ Functions
- DeepONet $\rightarrow$ Operators (branch-trunk)
- FNO $\rightarrow$ Operators (spectral)
- Next: Multi-scale, multi-physics

**Convergence of Fields:**

- Machine Learning
- Numerical Analysis
- Applied Mathematics
- Scientific Computing

**FNO represents a beautiful synthesis:**

Using physics-inspired architectures (Fourier)

$+$

Machine learning (neural networks)

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Fast, accurate operator learning for science and engineering

# Questions?

Thank you!

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**Interactive Demo:**

FNO Notebook